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Travelling waves in atomic models for phase-transforming materials and kinetic relations

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(joint work with Hartmut Schwetlick)

The aim is to prove the existence of travelling waves for discrete models of phase-transforming materials and derive so-called kinetic relations. The motivation is as follows. Consider the equations of motions of an elastic material,

$$(1) \quad u_{tt}(x) = \text{Div}(\sigma(Du(x))).$$

Here, u is the displacement field $u: \Omega \rightarrow \mathbb{R}^m$, with $\Omega \subset \mathbb{R}^n$; σ is the stress tensor. Let V denote the elastic energy density, then $\sigma(F) = \frac{\partial V}{\partial F}$. For phase transitions, V is commonly assumed to be non-convex, and σ is thus non-monotone. Equation (1) is consequently of elliptic-hyperbolic type. Our understanding of this ill-posed equation is at present very limited.

From an engineering viewpoint, this is not surprising. The ill-posed nature of Equation (1) is related to the motion of an interface between stable phases. There is no physical law describing the motion of such an interface as a function of the relevant forces.

It thus seems reasonable to study the motion of a single interface between two phases in detail. A moving interface is exposed to the so-called *configurational force* f , and we denote the velocity of the interface by c . A *kinetic relation* is a functional relationship between f and c , and will be expressed here in the form $f = f(c)$. We refer the reader to [6, 1] for more information on kinetic relations.

A number of successful models in engineering postulate a phenomenological kinetic relation to resolve the problem of being ill-posed. This obviously raises the question whether kinetic relations can be derived rigorously. A natural starting point is the atomic scale. Truskinovsky and Vainchtein obtained for such a model the existence of travelling waves [7] and derived quasicontinuum models from the microscopic picture [8]. The existence argument for waves on a bi-sided infinite chain of atom commonly relies on the so-called *causality principle for a steady-state solution* [5].

We aim to develop a simple approach for proving the existence of travelling waves in lattices, and derive kinetic relations. The precise setting is as follows. We consider a one-dimensional chain of atoms $\{q_j\}_{j \in \mathbb{Z}}$ on the real line. Neighbouring atoms are linked by a bistable spring with elastic potential V . The deformation of atom k is given by $u_k: \mathbb{R} \rightarrow \mathbb{R}$. The argument of the elastic potential V is the discrete strain, which is given by the difference of the deformations, $u_{k+1}(t) - u_k(t)$. The equations of motion are assumed to be governed by Newton's law. In suitable units, Newton's law reads

$$(2) \quad \ddot{u}_k(t) = V'(u_{k+1}(t) - u_k(t)) - V'(u_k(t) - u_{k-1}(t))$$

for every $k \in \mathbb{Z}$. This is a spatially discretized, one-dimensional version of Equation (1). Since the quest for rigorous kinetic relations requires a detailed understanding of the existence of travelling waves, we switch the travelling wave formulation

$$(3) \quad u_k(t) = u(k - ct) \text{ for } k \in \mathbb{Z}.$$

Then Equation (2) becomes

$$(4) \quad c^2 \ddot{u}(x) = V'(u(x+1) - u(x)) - V'(u(x) - u(x-1)).$$

We remark that this is the Euler-Lagrange function for the action functional

$$\phi(u) := \int_{\mathbb{R}} \left[\frac{1}{2} c^2 \dot{u}(t)^2 - V(u(t+1) - u(t)) \right] dt.$$

To describe martensitic phase transitions, the interaction potential V is assumed to be *nonconvex*. So far, a rigorous analysis seems to be confined to special form of V , namely a piecewise quadratic energy,

$$(5) \quad V(\epsilon) := \frac{1}{2} \min\{(\epsilon+1)^2, (\epsilon-1)^2\}$$

(here and below, we write $\epsilon := u(t+1) - u(t)$ for the discrete strain).

The aim is to investigate the existence of solutions to (4) with V given by (5). To ensure that both wells of the energy V are visited, we concentrate on heteroclinic waves with the strain distribution

$$\epsilon > 0 \text{ for } x > 0 \text{ and } \epsilon < 0 \text{ for } x < 0$$

(other ratios are possible, as discussed below). Of particular interest are subsonic waves, since kinetic relations can be shown to be relevant in this case. For V given in (5), the wave speed is 1. We develop a method to prove rigorously the existence of a solution to (4) for sufficiently large velocities below the wave speed 1. The main difficulty is that Fourier methods are not readily available, since singularities stemming from zeros of the dispersion relation have to be taken into account.

We remark that it is not hard to see that on a torus of length L , the existence of solutions with the strain distribution

$$(6) \quad \epsilon > 0 \text{ on } (0, \frac{L}{2}) \text{ and } \epsilon < 0 \text{ on } (\frac{L}{2}, L)$$

depends on the wave speed c : for some velocities c , a solution exists, while for other velocities nonexistence of a solution with strain distribution (6) can be proved.

For waves on the real line, it is possible to show that the solution satisfies the Rankine-Hugoniot conditions. Furthermore, the configurational force f can be shown to be zero, so that $f(c) = 0$ is the desired kinetic relation. A closer analysis reveals that the symmetry of the solution, imposed by the sign condition (6), leads to the vanishing configurational force. It is expected that asymmetric distributions will give rise to non-vanishing kinetic relations; the waves with asymmetric sign distribution are likely to have an interpretation as suitable limits of waves on a torus as $L \rightarrow \infty$, as in the symmetric case.

We close this report by pointing out that the interest in lattice models such as Equation (4) goes beyond the realm of phase transitions. Indeed, Equation (4) is

an instance of a so-called *lattice differential equation*. Many problems, such models of crystal lattices, photonic structures, and Josephson junctions, can be described by lattice differential equations as well. There are a number of mathematical problems associated with lattice differential equations in general. A number of interesting papers [2, 3, 4] give a good insight into this field.

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